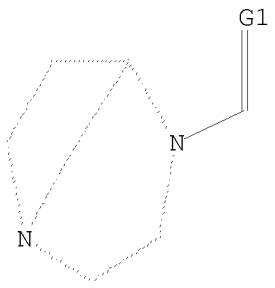
```
=> d his

     (FILE 'HOME' ENTERED AT 14:23:16 ON 01 FEB 2008)

     FILE 'REGISTRY' ENTERED AT 14:23:32 ON 01 FEB 2008

     FILE 'CAPLUS' ENTERED AT 14:39:22 ON 01 FEB 2008

     FILE 'REGISTRY' ENTERED AT 14:41:05 ON 01 FEB 2008

     FILE 'CAPLUS' ENTERED AT 14:44:42 ON 01 FEB 2008

     FILE 'REGISTRY' ENTERED AT 14:57:40 ON 01 FEB 2008
L1               STRUCTURE UPLOADED
L2             1 S L1
L3               STRUCTURE UPLOADED
L4             1 S L3
L5            50 S L3 SSS FUL

     FILE 'CAPLUS' ENTERED AT 14:59:46 ON 01 FEB 2008
L6            11 S L5

=> d l3
L3 HAS NO ANSWERS
L3               STR
```




```
G1 O,S
```

Structure attributes must be viewed using STN Express query preparation.

```
=> d ibib abs hitstr total
```

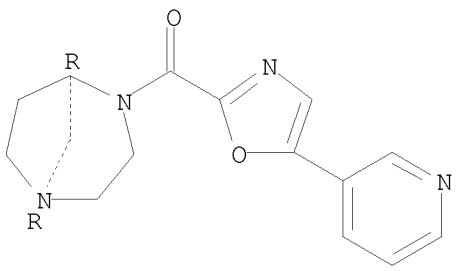
L6 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:996358 CAPLUS
DOCUMENT NUMBER: 147:461507
TITLE: Use of trifluoroacetic acid to quantify small, polar compounds in rat plasma during discovery-phase pharmacokinetic evaluation
AUTHOR(S): Bock, M. J.; Neilson, K. L.; Dudley, A.
CORPORATE SOURCE: Discovery DMPK, AstraZeneca, Wilmington, DE, 19803, USA
SOURCE: Journal of Chromatography, B: Analytical Technologies in the Biomedical and Life Sciences (2007), 856(1-2), 165-170
CODEN: JCBAAI; ISSN: 1570-0232
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Although it is accepted that trifluoroacetic acid (TFA) can cause suppression of an analyte during LC/MS anal., this paper presents a relatively sensitive gradient method that uses a TFA mobile phase for the improved quantification of small, polar drug-like compds. The described method was developed in a discovery drug metabolism and pharmacokinetics (DMPK) laboratory for the screening measurement of compound concns. to calculate PK parameters and CNS exposure of compds. from a chemical series that had poor chromatog. under generic methods using formic acid mobile phase. The samples were collected by a Culex automated sampling unit, and the plasma proteins were precipitated by a Tecan robot in 96-well plates. After centrifugation, the supernatant was removed, dried down using a SPE-Dry unit, and the samples were reconstituted in aqueous buffer on the robot. The samples were analyzed on an Agilent LC/MSD using a 5-min gradient on a 5 cm Ph column. No addnl. steps, such as the "TFA-fix", were necessary. Although sample batches were analyzed over 6 h, no drift or degradation of signal was observed The improved chromatog. resulted in a method that was selective, rugged, and had a dynamic range from 5 to 20,000 nM, which was sufficient to quantitate low volume, serial plasma samples collected out to 8 h postdose.

IT 857521-69-8
RL: ANT (Analyte); PKT (Pharmacokinetics); ANST (Analytical study); BIOL (Biological study)
(use of trifluoroacetic acid to quantify small, polar compds. in rat plasma during discovery-phase pharmacokinetic evaluation)

RN 857521-69-8 CAPLUS
CN Methanone, (1R,5R)-1,4-diazabicyclo[3.2.1]oct-4-yl[5-(3-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)

Absolute stereochemistry.

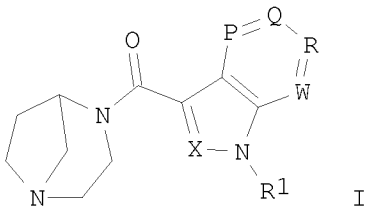


REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

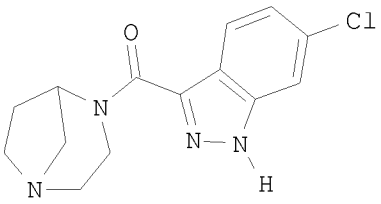
L6 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:637812 CAPLUS
DOCUMENT NUMBER: 143:133407
TITLE: Preparation of 1,4-diazabicyclo[3.2.1]octanecarboxamides as ligands for nicotinic receptors, especially α4β2 and α7 subunits, for treating central nervous system diseases
INVENTOR(S): Galli, Frederic; Leclerc, Odile; Lochead, Alistoir W.
PATENT ASSIGNEE(S): Sanofi-Synthelabo S.A., Fr.
SOURCE: Fr. Demande, 22 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2865208	A1	20050722	FR 2004-390	20040116
AU 2005212867	A1	20050825	AU 2005-212867	20050107
CA 2549954	A1	20050825	CA 2005-2549954	20050107
WO 2005077955	A1	20050825	WO 2005-FR27	20050107
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1709052	A1	20061011	EP 2005-717375	20050107
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, BA, HR, IS, YU				
CN 1946726	A	20070411	CN 2005-80002630	20050107
BR 2005006879	A	20070612	BR 2005-6879	20050107
JP 2007517838	T	20070705	JP 2006-548338	20050107
IN 2006KN01850	A	20070511	IN 2006-KN1850	20060703
US 2007155749	A1	20070705	US 2006-456345	20060710
MX 2006PA07984	A	20061019	MX 2006-PA7984	20060712
KR 2007017990	A	20070213	KR 2006-714266	20060714
NO 2006003666	A	20061011	NO 2006-3666	20060814
PRIORITY APPLN. INFO.:			FR 2004-390 A	20040116
			WO 2005-FR27 W	20050107

OTHER SOURCE(S): MARPAT 143:133407
GI



I



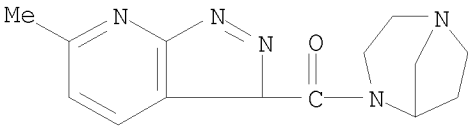
II

AB Title compds. I [wherein X = N, CR2, P = CR3, Q = CR4; R = CR5; W = CR6, or one of P, Q, R, W = N; R1, R2 = independently H, alkyl; R3, R4, R5, R6 = independently H, halo, alkyl, alkoxy, NO2, NH2 and derivs., CF3, CN, NHCO2H and derivs., OH and derivs., SH and derivs., CO2H and derivs., CONH2 and derivs., etc.; R3CCR4, R4CCR5, R5CCR6 = (un)substituted hetero/aromatic 6-membered; their free bases and salts of addition with acids] were prepared as CNS agents, and specifically as ligands of nicotinic receptor. The compds. were tested against nicotinic receptors with the α4β2 subunit or with the α7 subunit. Thus, reacting 3-iodo-6-chloro-1H-indazole with 1,4-diazabicyclo[3.2.1]octane and CO in the presence of TEA/DMF at 70° for 8 h gave II•HCl (m.p. = 285-286°). In tests for specific binding to isolated rat cerebral nicotinic receptors having either α4β2 or α7 subunits, compds. I displayed IC50 values in the ranges of 1-10 μM and 0.01-0.1 μM, resp. I showed selectivity for the α7 receptor subtype.

IT 858628-83-8P, 3-[(1,4-Diazabicyclo[3.2.1]oct-4-yl)carbonyl]-6-methyl-1H-pyrazolo[3,4-b]pyridine dihydrobromide 858628-85-0P, 3-[(1,4-Diazabicyclo[3.2.1]oct-4-yl)carbonyl]-1H-indazole monohydrochloride 858628-87-2P, 6-Chloro-3-[(1,4-diazabicyclo[3.2.1]oct-4-yl)carbonyl]-1H-indazole monohydrobromide 858628-89-4P, 3-[(1,4-Diazabicyclo[3.2.1]oct-4-yl)carbonyl]-5-fluoro-1H-indazole dihydrobromide 858628-91-8P 858628-94-1P 858628-96-3P 858628-98-5P 858629-01-3P 858638-38-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(nicotinic receptor α7 subunit ligand; preparation of 1,4-diazabicyclo[3.2.1]octanecarboxamides as ligands for nicotinic receptors, especially α4β2 and α7 subunits, for treating central nervous system diseases)

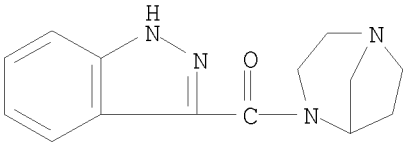
RN 858628-83-8 CAPLUS

CN 1,4-Diazabicyclo[3.2.1]octane, 4-[(6-methyl-3H-pyrazolo[3,4-b]pyridin-3-yl)carbonyl]-, dihydrobromide (9CI) (CA INDEX NAME)



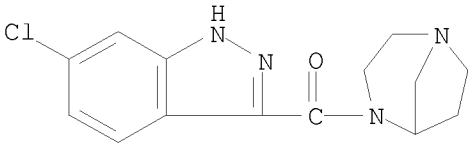
● 2 HBr

RN 858628-85-0 CAPLUS
CN 1,4-Diazabicyclo[3.2.1]octane, 4-(1H-indazol-3-ylcarbonyl)-, monohydrochloride (9CI) (CA INDEX NAME)



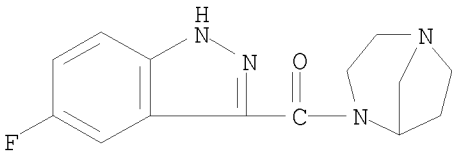
● HCl

RN 858628-87-2 CAPLUS
CN 1,4-Diazabicyclo[3.2.1]octane, 4-[(6-chloro-1H-indazol-3-yl)carbonyl]-, monohydrobromide (9CI) (CA INDEX NAME)



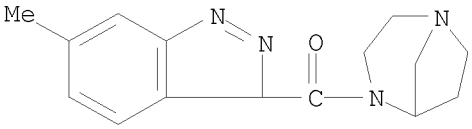
● HBr

RN 858628-89-4 CAPLUS
CN 1,4-Diazabicyclo[3.2.1]octane, 4-[(5-fluoro-1H-indazol-3-yl)carbonyl]-, dihydrobromide (9CI) (CA INDEX NAME)



●2 HBr

RN 858628-91-8 CAPLUS
CN 1,4-Diazabicyclo[3.2.1]octane, 4-[(6-methyl-3H-indazol-3-yl)carbonyl]-, hydrobromide (9CI) (CA INDEX NAME)

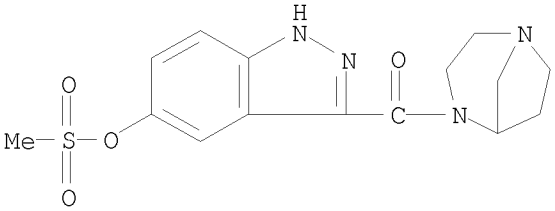


●x HBr

RN 858628-94-1 CAPLUS
CN 1,4-Diazabicyclo[3.2.1]octane, 4-[[5-[(methylsulfonyl)oxy]-1H-indazol-3-yl]carbonyl]-, ethanedioate (9CI) (CA INDEX NAME)

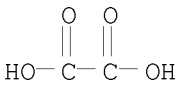
CM 1

CRN 858628-93-0
CMF C15 H18 N4 O4 S

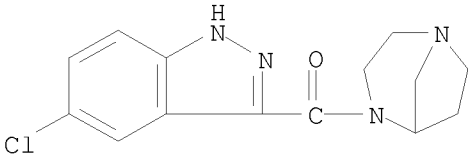


CM 2

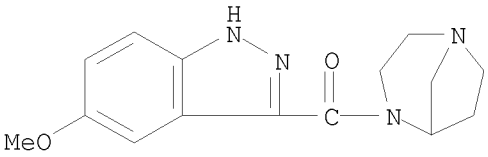
CRN 144-62-7
CMF C2 H2 O4



RN 858628-96-3 CAPLUS
CN 1,4-Diazabicyclo[3.2.1]octane, 4-[(5-chloro-1H-indazol-3-yl)carbonyl]-
(9CI) (CA INDEX NAME)



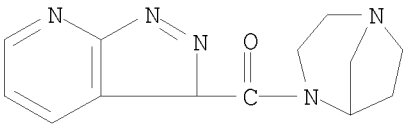
RN 858628-98-5 CAPLUS
CN 1,4-Diazabicyclo[3.2.1]octane, 4-[(5-methoxy-1H-indazol-3-yl)carbonyl]-
(9CI) (CA INDEX NAME)



RN 858629-01-3 CAPLUS
CN 1,4-Diazabicyclo[3.2.1]octane, 4-(3H-pyrazolo[3,4-b]pyridin-3-ylcarbonyl)-
, ethanedioate (9CI) (CA INDEX NAME)

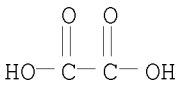
CM 1

CRN 858629-00-2
CMF C13 H15 N5 O

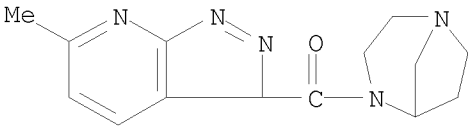


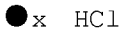
CM 2

CRN 144-62-7
CMF C2 H2 O4



RN 858638-38-7 CAPLUS
CN 1,4-Diazabicyclo[3.2.1]octane, 4-[(6-methyl-3H-pyrazolo[3,4-b]pyridin-3-yl)carbonyl]-, hydrochloride (9CI) (CA INDEX NAME)



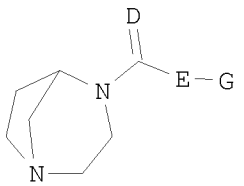


REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

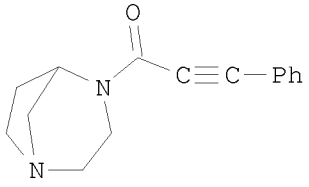
L6 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:588985 CAPLUS
DOCUMENT NUMBER: 143:115572
TITLE: Preparation of 1,3-ethanopiperazines as nicotinic acetylcholine receptor ligands
INVENTOR(S): Ernst, Glen; Frietze, William; Jacobs, Robert; Phillips, Eifion
PATENT ASSIGNEE(S): Astrazeneca AB, Swed.
SOURCE: PCT Int. Appl., 23 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2005061511	A1	20050707	WO 2004-SE1942		20041220
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW					
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
EP 1699802	A1	20060913	EP 2004-809115		20041220
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS					
CN 1902204	A	20070124	CN 2004-80038236		20041220
JP 2007515480	T	20070614	JP 2006-546910		20041220
IN 2006DN03176	A	20070824	IN 2006-DN3176		20060602
US 2007244097	A1	20071018	US 2007-583585		20070410
PRIORITY APPLN. INFO.:			US 2003-531644P	P	20031222
			WO 2004-SE1942	W	20041220

OTHER SOURCE(S): MARPAT 143:115572
GI



I



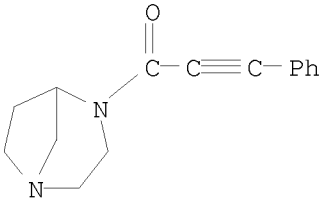
II

AB Title compds. I [D = O, S, N(R1)2; E = C(R1)2C(R1)2, CR1=CR1, C(R1)2O, etc.; G = 5- or 6-membered aromatic or heteroarom. ring; R1 = H, halo, alkyl,

etc.] and their pharmaceutically acceptable salts were prepared For example, coupling of phenylpropynoic acid and 1,4-diazabicyclo[3.2.1]octane dihydrochloride afforded ethanopiperazine II. In nicotinic receptor α7 affinity binding assays, compds. I exhibited specific binding of 75% (sic).

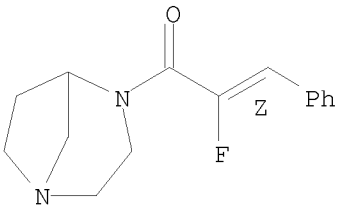
IT 857334-56-6P 857334-57-7P 857334-58-8P
857334-59-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of ethanopiperazines as nicotinic acetylcholine receptor ligands)

RN 857334-56-6 CAPLUS
CN 1,4-Diazabicyclo[3.2.1]octane, 4-(1-oxo-3-phenyl-2-propynyl)- (9CI) (CA INDEX NAME)



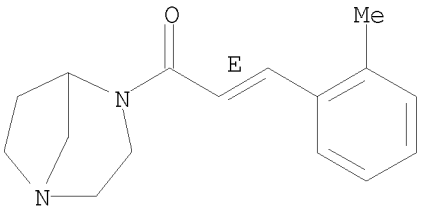
RN 857334-57-7 CAPLUS
CN 1,4-Diazabicyclo[3.2.1]octane, 4-[(2Z)-2-fluoro-1-oxo-3-phenyl-2-propenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



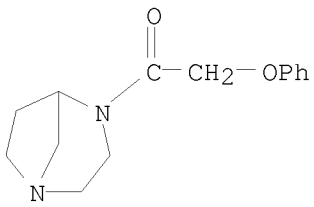
RN 857334-58-8 CAPLUS
CN 1,4-Diazabicyclo[3.2.1]octane, 4-[(2E)-3-(2-methylphenyl)-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 857334-59-9 CAPLUS

CN 1,4-Diazabicyclo[3.2.1]octane, 4-(phenoxyacetyl)- (9CI) (CA INDEX NAME)

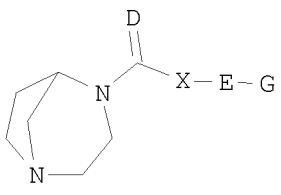


REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

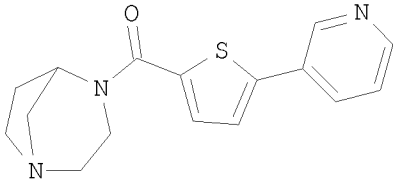
L6 ANSWER 4 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:588983 CAPLUS
DOCUMENT NUMBER: 143:115571
TITLE: Preparation of 1,3-ethanopiperazines as nicotinic acetylcholine receptor ligands
INVENTOR(S): Ernst, Glen; Frietze, William; Jacobs, Robert; Phillips, Eifion
PATENT ASSIGNEE(S): Astrazeneca AB, Swed.
SOURCE: PCT Int. Appl., 40 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2005061510	A1	20050707	WO 2004-SE1941		20041220
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW					
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
AU 2004303738	A1	20050707	AU 2004-303738		20041220
CA 2550655	A1	20050707	CA 2004-2550655		20041220
EP 1699801	A1	20060913	EP 2004-809114		20041220
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, BA, HR, IS, YU					
CN 1918166	A	20070221	CN 2004-80041294		20041220
BR 2004017946	A	20070417	BR 2004-17946		20041220
JP 2007515479	T	20070614	JP 2006-546909		20041220
IN 2006DN03172	A	20070803	IN 2006-DN3172		20060602
MX 2006PA07027	A	20060831	MX 2006-PA7027		20060619
NO 2006003354	A	20060921	NO 2006-3354		20060719
US 2007249588	A1	20071025	US 2007-583576		20070326
PRIORITY APPLN. INFO.:			US 2003-531710P	P	20031222
			WO 2004-SE1941	W	20041220

OTHER SOURCE(S): MARPAT 143:115571
GI



I



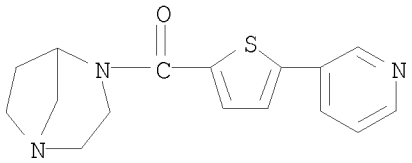
II

AB Title compds. I [D = O, S, N(R1)2; X = Ar1; Ar1 = 5- or 6-membered aromatic or heteroarom. ring with provisos; E = single bond, O, S, etc.; G = H, alkoxy, 5- or 6-membered aromatic or heteroarom. ring, etc.;] and their pharmaceutically acceptable salts were prepared For example, coupling of 1,4-diazabicyclo[3.2.1]octane dihydrochloride and 5-(2-pyridyl)thiophene-2-carboxylic acid afforded ethanopiperazine II in 60% yield. In nicotinic receptor α7 affinity binding assays, compds. I exhibited specific binding of 75% (sic).

IT 857334-62-4P 857334-63-5P 857334-64-6P
857334-65-7P 857334-66-8P 857334-67-9P
857334-68-0P 857334-69-1P 857334-70-4P
857334-71-5P 857334-72-6P 857334-73-7P
857334-74-8P 857334-75-9P 857334-76-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of ethanopiperazines as nicotinic acetylcholine receptor ligands)

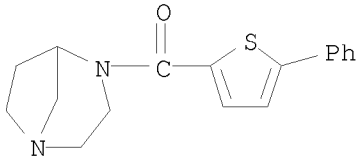
RN 857334-62-4 CAPLUS

CN 1,4-Diazabicyclo[3.2.1]octane, 4-[[5-(3-pyridinyl)-2-thienyl]carbonyl]- (9CI) (CA INDEX NAME)



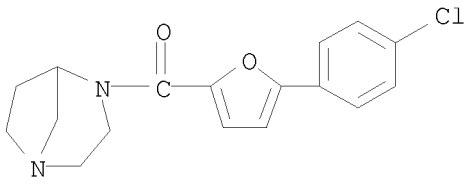
RN 857334-63-5 CAPLUS

CN 1,4-Diazabicyclo[3.2.1]octane, 4-[(5-phenyl-2-thienyl)carbonyl]- (9CI) (CA INDEX NAME)

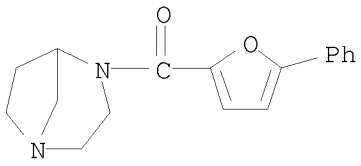


RN 857334-64-6 CAPLUS

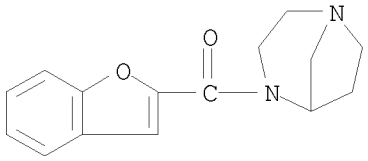
CN 1,4-Diazabicyclo[3.2.1]octane, 4-[[5-(4-chlorophenyl)-2-furanyl]carbonyl]- (9CI) (CA INDEX NAME)



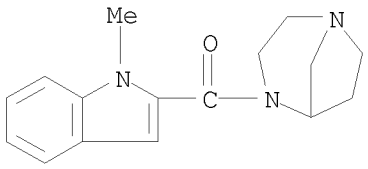
RN 857334-65-7 CAPLUS
CN 1,4-Diazabicyclo[3.2.1]octane, 4-[(5-phenyl-2-furanyl)carbonyl]- (9CI) (CA INDEX NAME)



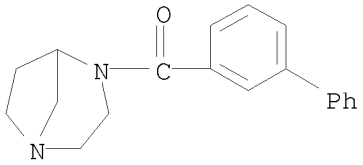
RN 857334-66-8 CAPLUS
CN 1,4-Diazabicyclo[3.2.1]octane, 4-(2-benzofuranylcarbonyl)- (9CI) (CA INDEX NAME)



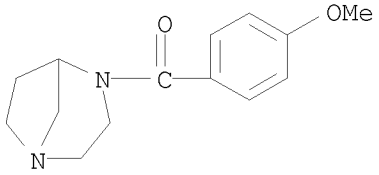
RN 857334-67-9 CAPLUS
CN 1,4-Diazabicyclo[3.2.1]octane, 4-[(1-methyl-1H-indol-2-yl)carbonyl]- (9CI) (CA INDEX NAME)



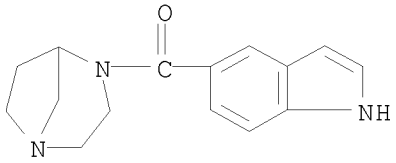
RN 857334-68-0 CAPLUS
CN 1,4-Diazabicyclo[3.2.1]octane, 4-([1,1'-biphenyl]-3-ylcarbonyl)- (9CI) (CA INDEX NAME)



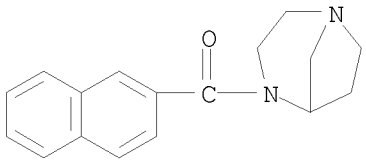
RN 857334-69-1 CAPLUS
CN 1,4-Diazabicyclo[3.2.1]octane, 4-(4-methoxybenzoyl)- (9CI) (CA INDEX NAME)



RN 857334-70-4 CAPLUS
CN 1,4-Diazabicyclo[3.2.1]octane, 4-(1H-indol-5-ylcarbonyl)- (9CI) (CA INDEX NAME)

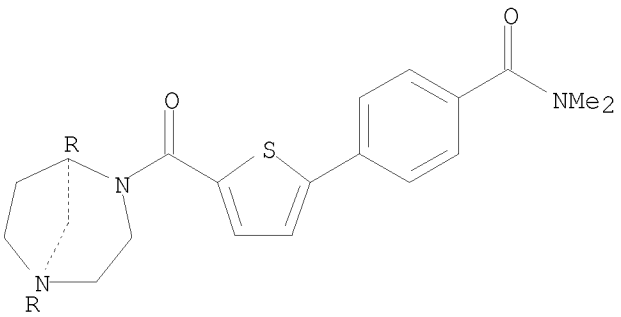


RN 857334-71-5 CAPLUS
CN 1,4-Diazabicyclo[3.2.1]octane, 4-(2-naphthalenylcarbonyl)- (9CI) (CA INDEX NAME)



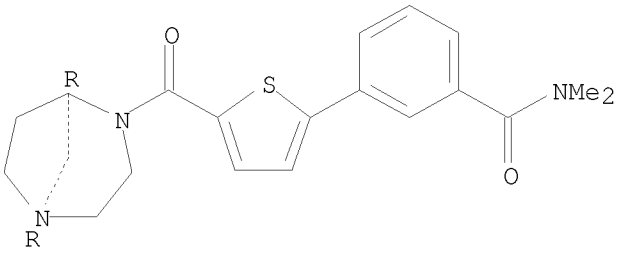
RN 857334-72-6 CAPLUS
CN Benzamide, 4-[5-[(1R,5R)-1,4-diazabicyclo[3.2.1]oct-4-ylcarbonyl]-2-thienyl]-N,N-dimethyl- (CA INDEX NAME)

Absolute stereochemistry.



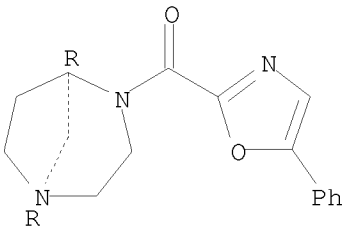
RN 857334-73-7 CAPLUS
CN Benzamide, 3-[5-[(1R,5R)-1,4-diazabicyclo[3.2.1]oct-4-ylcarbonyl]-2-thienyl]-N,N-dimethyl- (CA INDEX NAME)

Absolute stereochemistry.



RN 857334-74-8 CAPLUS
CN 1,4-Diazabicyclo[3.2.1]octane, 4-[(5-phenyl-2-oxazolyl)carbonyl]-, monohydrochloride, (1R,5R)- (9CI) (CA INDEX NAME)

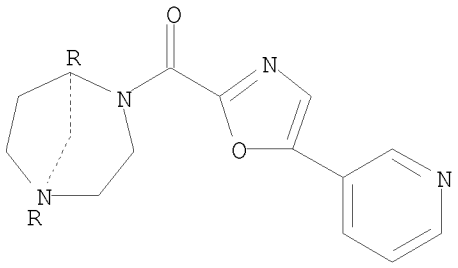
Absolute stereochemistry.



● HCl

RN 857334-75-9 CAPLUS
CN 1,4-Diazabicyclo[3.2.1]octane, 4-[[5-(3-pyridinyl)-2-oxazolyl]carbonyl]-, dihydrochloride, (1R,5R)- (9CI) (CA INDEX NAME)

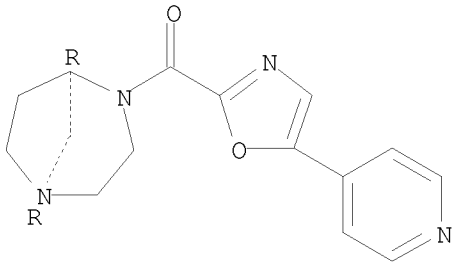
Absolute stereochemistry.



●2 HCl

RN 857334-76-0 CAPLUS
CN 1,4-Diazabicyclo[3.2.1]octane, 4-[[5-(4-pyridinyl)-2-oxazolyl]carbonyl]-, dihydrochloride, (1R,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



●2 HCl

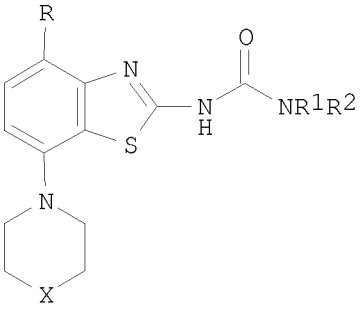
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 5 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:472390 CAPLUS
DOCUMENT NUMBER: 139:53026
TITLE: Preparation of ureidobenzothiazoles as adenosine receptor ligands
INVENTOR(S): Flohr, Alexander; Jakob-Roetne, Roland; Norcross, Roger David; Riemer, Claus
PATENT ASSIGNEE(S): F. Hoffmann-La Roche Ag, Switz.
SOURCE: PCT Int. Appl., 42 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003049741	A1	20030619	WO 2002-EP13761	20021205
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2003149036	A1	20030807	US 2002-308338	20021203
US 6727247	B2	20040427		
CA 2469596	A1	20030619	CA 2002-2469596	20021205
AU 2002356626	A1	20030623	AU 2002-356626	20021205
AU 2002356626	B2	20071129		
BR 2002014825	A	20040914	BR 2002-14825	20021205
EP 1455792	A1	20040915	EP 2002-804578	20021205
EP 1455792	B1	20070418		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
CN 1602196	A	20050330	CN 2002-824654	20021205
JP 2005516006	T	20050602	JP 2003-550790	20021205
AT 359792	T	20070515	AT 2002-804578	20021205
ES 2283652	T3	20071101	ES 2002-804578	20021205
RU 2311905	C2	20071210	RU 2004-121166	20021205
US 2004229893	A1	20041118	US 2003-691770	20031023
US 7019001	B2	20060328		
MX 2004PA05444	A	20041011	MX 2004-PA5444	20040604

PRIORITY APPLN. INFO.:	EP 2001-129228	A	20011210
	US 2002-308338	A3	20021203
	WO 2002-EP13761	W	20021205

OTHER SOURCE(S): MARPAT 139:53026
GI



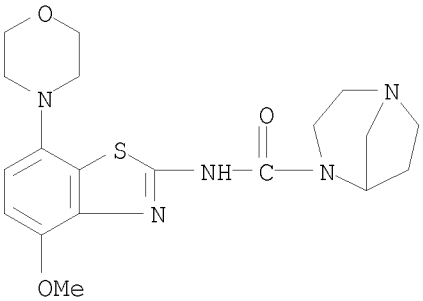
I

AB Title compds. [I; R = alkoxy, halo; R1, R2 = H, alkyl, cycloalkyl, tetrahydropyran-4-yl; R1R2N = (substituted) 2-oxa-5-azabicyclo[2.2.1]heptyl, 3-endo-hydroxy-8-azabicyclo[3.2.1]octyl, 2-azabicyclo[2.2.2]octyl, 1-oxo-2,8-diazaspiro[4.5]decyl, 3-azaspiro[5.5]undecyl, 8-azaspiro[4.5]decyl, 1-oxa-8-azaspiro[4.5]decyl, 1,8,8-trimethyl-3-azabicyclo[3.2.1]octyl, 1,4-oxazepanyl, 2-oxa-5-azabicyclo[2.2.2]octyl, 8-oxa-3-azabicyclo[3.2.1]octyl, 1,4-diazabicyclo[3.2.1]octyl, 2-azabicyclo[2.2.1]heptyl, 3-azabicyclo[3.2.1]octyl, piperazinyl, piperidin-1-yl; X = O, CH2; n = 0-4], were prepared Thus, 4-methoxy-7-morpholin-4-ylbenzothiazol-2-ylamine in CH2Cl2 was treated with pyridine and Ph chloroformate and the resulting solution stirred for 45 min at ambient temperature; (1S,4S)-2-oxa-5-azabicyclo[2.2.1]heptane was added and the mixture stirred at ambient temperature for 15 min and at 40° for 2.5 h. to give (1S,4S)-2-oxa-5-azabicyclo[2.2.1]heptane-5-carboxylic acid (4-methoxy-7-morpholin-4-ylbenzothiazol-2-yl)amide. This bound to human A2a receptors with pKi = 8.5.

IT 546093-56-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of ureidobenzothiazoles as adenosine receptor ligands)

RN 546093-56-5 CAPLUS

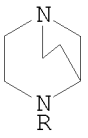
CN 1,4-Diazabicyclo[3.2.1]octane-4-carboxamide, N-[4-methoxy-7-(4-morpholinyl)-2-benzothiazolyl]- (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

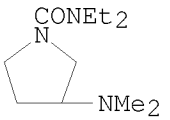
L6 ANSWER 6 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1977:527018 CAPLUS
DOCUMENT NUMBER: 87:127018
ORIGINAL REFERENCE NO.: 87:20081a,20084a
TITLE: Antifilarial agents. 3-Aminopyrrolidine and 1,4-diazabicyclo[3.2.1]octane derivatives as analogs of diethylcarbamazine
AUTHOR(S): Sturm, Priscilla A.; Cory, Michael; Henry, David W.; McCall, J. W.; Ziegler, J. B.
CORPORATE SOURCE: Bio-Org. Chem. Dep., Stanford Res. Inst., Menlo Park, CA, USA
SOURCE: Journal of Medicinal Chemistry (1977), 20(10), 1333-7
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 87:127018
GI

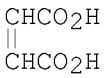


$_n$HCl

I, R=H, $_n$=2

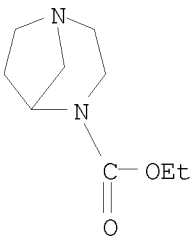
II, R=CONEt$_2$, $_n$=1





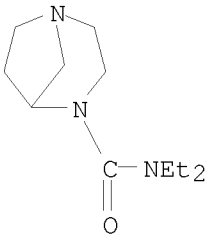
III

AB Four 3-aminopyrrolidine acyl derivs. and 1,4-diazabicyclo[3.2.1]octane-2HCl (I) [5492-61-5] and 2 acyl derivs. were prepared, of which all but I had significant activity in the Litomosoides carinii gerbil test system but had no effect on adult worms. The most active diazabicyclo compound, II [60137-50-0], was prepared from 2-(2-hydroxyethyl)pyrazine [6705-31-3] by hydrogenation, chlorination, ring closure, and acylation. The most active aminopyrrolidine, III [64021-90-5], was prepared from 3-pyrrolidinol [40499-83-0] by acylation, chlorination, reaction with benzylamine, methylation, debenzylation, and methylation. Structure-activity relations are discussed, including the effects of conformation and positions of pharmacophores.
IT 60137-49-7P 60137-50-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and anthelmintic activity of)
RN 60137-49-7 CAPLUS
CN 1,4-Diazabicyclo[3.2.1]octane-4-carboxylic acid, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)



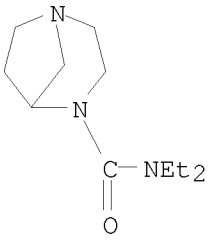
● HCl

RN 60137-50-0 CAPLUS
CN 1,4-Diazabicyclo[3.2.1]octane-4-carboxamide, N,N-diethyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

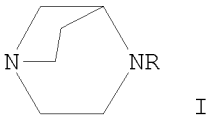
L6 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1977:527003 CAPLUS
DOCUMENT NUMBER: 87:127003
ORIGINAL REFERENCE NO.: 87:20077a,20080a
TITLE: Antifilarial agents. 1,2-Cyclobutanediamines as analogs of diethylcarbamazine. Status of structure-activity relations among diethylcarbamazine analogs
AUTHOR(S): Sturm, Priscilla A.; Cory, Michael; Henry, David W.; McCall, J. W.; Ziegler, J. B.
CORPORATE SOURCE: Coll. Vet. Med., Univ. Georgia, Athens, GA, USA
SOURCE: Journal of Medicinal Chemistry (1977), 20(10), 1327-33
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
AB One cis- and 7 trans-1,2-cyclobutanediamines with N-methyl and N-acyl substituents were prepared by monoacylating the appropriate diamine followed by reductive methylation. None of the compds. was active against Litomosoides carinii in the gerbil. Inactivity is discussed in terms of pharmacophore configurations. Structure-activity relations for 24 addnl. diethylcarbamazine [90-89-1] analogs are discussed.
IT 63574-73-2
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(anthelmintic activity of, structure in relation to)
RN 63574-73-2 CAPLUS
CN 1,4-Diazabicyclo[3.2.1]octane-4-carboxamide, N,N-diethyl- (CA INDEX NAME)



L6 ANSWER 8 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1976:494404 CAPLUS
DOCUMENT NUMBER: 85:94404
ORIGINAL REFERENCE NO.: 85:15129a,15132a
TITLE: 1,4-Diazabicyclo[3.2.1]octanes
INVENTOR(S): Henry, David W.; Sturm, Priscilla A.
PATENT ASSIGNEE(S): Stanford Research Institute, USA
SOURCE: U.S., 3 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3954766	A	19760504	US 1975-594510	19750709
PRIORITY APPLN. INFO.:			US 1975-594510 A	19750709

GI



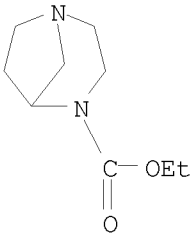
I

AB Diazabicyclooctanes (I; R = EtOCO, Et2NCO), useful as antifilarial agents as indicated by tests against Litomosoides carinii in gerbils, were prepared by acylation of I (R = H) (II) with EtOCOCl and Et2NCOCl; the compds. were isolated as HCl salts. II was prepared by hydrogenating 2-(2-hydroxyethyl)pyrazine with PtO2 catalyst, treating the product with SOCl2, and cyclizing the resultant 2-(2-chloroethyl)piperazine with aqueous NaOH.

IT 60137-49-7P 60137-50-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, for use as antifilarial agent)

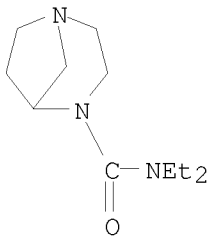
RN 60137-49-7 CAPLUS

CN 1,4-Diazabicyclo[3.2.1]octane-4-carboxylic acid, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)



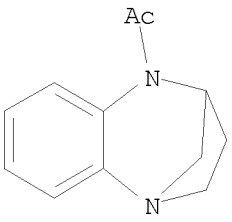
● HCl

RN 60137-50-0 CAPLUS
CN 1,4-Diazabicyclo[3.2.1]octane-4-carboxamide, N,N-diethyl-, monohydrochloride (9CI) (CA INDEX NAME)

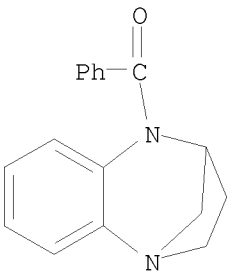


● HCl

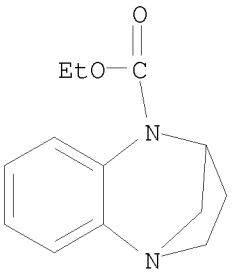
L6 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1973:124539 CAPLUS
DOCUMENT NUMBER: 78:124539
ORIGINAL REFERENCE NO.: 78:20011a,20014a
TITLE: Synthesis of benzo[b]-1,4-diazabicyclo[3.2.1]octane
AUTHOR(S): Cunningham, Howard C.; Day, Allan R.
CORPORATE SOURCE: Dep. Chem., Univ. Pennsylvania, Philadelphia, PA, USA
SOURCE: Journal of Organic Chemistry (1973), 38(6), 1225-7
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Synthesis of benzo [b]-1,4-diazabicyclo[3.2.1]octane (I), from 3-ethoxy-carbonylmethylene-2-quinoxalone is described. Spectral data are used to prove its structure.
IT 37931-46-7P 37931-47-8P 37931-48-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 37931-46-7 CAPLUS
CN 1,4-Methano-1H-1,5-benzodiazepine, 5-acetyl-2,3,4,5-tetrahydro- (9CI) (CA INDEX NAME)



RN 37931-47-8 CAPLUS
CN 1,4-Methano-1H-1,5-benzodiazepine, 5-benzoyl-2,3,4,5-tetrahydro- (9CI) (CA INDEX NAME)



RN 37931-48-9 CAPLUS
CN 1,4-Methano-1H-1,5-benzodiazepine-5(2H)-carboxylic acid, 3,4-dihydro-, ethyl ester (9CI) (CA INDEX NAME)


O
EtO
C
N
N

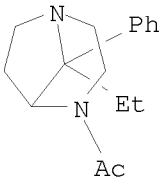
L6 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1972:113167 CAPLUS
DOCUMENT NUMBER: 76:113167
ORIGINAL REFERENCE NO.: 76:18277a,18280a
TITLE: Bridged bicyclic compounds. 6-Phenyl-6-ethyl-1-aza-4-oxabicyclo[3.2.1]octan-3-one and 8-phenyl-8-ethyl-1,4-diazabicyclo[3.2.1]octan-3-one
AUTHOR(S): Hirshfeld, A.; Taub, W.; Glotter, E.
CORPORATE SOURCE: Dep. Chem., Weizmann Inst. Sci., Rehovot, Israel
SOURCE: Tetrahedron (1972), 28(5), 1275-87
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 76:113167

AB Lactonization of the stereoisomeric N-(carboxymethyl)-4-phenyl-4-ethylpyrrolidin-3-ols as well as of the corresponding Me and Et esters and of their 3-acetates afforded the bicyclic lactone, 6-phenyl-6-ethyl-1-aza-4-oxabicyclo[3.2.1]octan-3-one. Reductive cyclization of N-(carbethoxymethyl)-2-phenyl-2-ethylpyrrolidin-3-one oxime yielded the bicyclic lactam, 8-phenyl-8-ethyl-1,4-diazabicyclo-[3.2.1]octan-3-one.

IT 35729-86-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 35729-86-3 CAPLUS
CN 1,4-Diazabicyclo[3.2.1]octane, 4-acetyl-8-ethyl-8-phenyl-, compd. with 2,4,6-trinitrophenol (1:1) (9CI) (CA INDEX NAME)

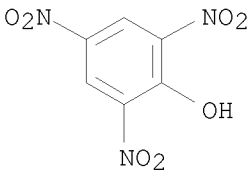
CM 1

CRN 46939-11-1
CMF C16 H22 N2 O



CM 2

CRN 88-89-1
CMF C6 H3 N3 O7



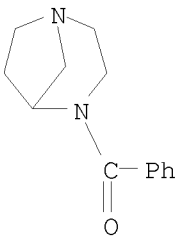
L6 ANSWER 11 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1966:27623 CAPLUS
DOCUMENT NUMBER: 64:27623
ORIGINAL REFERENCE NO.: 64:5115d-g
TITLE: 1,3-Ethanopiperazine and derivatives
PATENT ASSIGNEE(S): Merck & Co., Inc.
SOURCE: 9 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
NL 6501367		19650804	NL 1965-1367	19650203
US 3281423			US	
PRIORITY APPLN. INFO.:			US	19640203

AB 2-(2-Chloroethyl)piperazine (I) was treated with NaOH to give 1,3-ethanopiperazine (II), which was possibly acylated or alkylated at the 4-C. Thus, 10 g. 2-(2-hydroxyethyl)pyrazine was hydrogenated in 150 cc. MeOH at room temperature, under a H pressure of 2.8 kg./cm.2, in the presence of 2.5 g. Pt2O for 20 hrs., filtered off, and the filtrate distilled in vacuo to give a residue of 2-(2-hydroxyethyl)piperazine (III), which gave by reaction with an excess of HCl in MeOH, a precipitate of III.2HCl, m. .apprx.210°. SOCl2 (100 cc.) was added at -40° in 3-cc. portions to 20 g. III. The reaction mixture was refluxed 5.5 hrs., cooled to room temperature, and filtered. The residue was dried to give after precipitation from acetone I.2HCl (IV), m. 348-50°. A suspension of 60 g. IV in 45 cc. water was cooled and treated with 45 g. NaOH in 45 cc. water. The mixture was extracted 5 times with CHCl3, and the exts. were dried over Na2SO4 and evaporated in vacuo. The residue was distilled in the presence of NaOH at 3 mm. and <100° to give II. Reaction of II with excess HCl in MeOH yielded II.2HCl, m. 348°. A solution of 0.5 g. II in 3 cc. 10% NaOH solution was treated with 5 times 0.2 cc. BzCl. The solution was extracted 3 times with 5 cc. CHCl3. The exts. were dried on Na2SO4, evaporated in vacuo, and crystallized 2 times from ether, to give the 4-benzoyl homolog of II (V), m. 95-7°. MeI (14.2 g.) was added slowly with stirring to a solution of 11.3 g. II in 15 cc. acetone, and the mixture refluxed 2 hrs. and dried in vacuo. An aqueous alkaline solution of the residue was extracted 5 times with 10 cc. CHCl3. The exts. were dried over Na2SO4, evaporated, and distilled in vacuo. The fraction b20 67-70° was the 4-methyl homolog of II (VI). II, V, and VI are veterinary anthelmintics.

IT 5167-10-2P, 1,4-Diazabicyclo[3.2.1]octane, 4-benzoyl-
RL: PREP (Preparation)
(preparation of)

RN 5167-10-2 CAPLUS
CN 1,4-Diazabicyclo[3.2.1]octane, 4-benzoyl- (7CI, 8CI) (CA INDEX NAME)


N
N
C
Ph
O

=>